

Modelling Slag Viscosities on the Basis of the HotVeGas Oxide Database

GUIXUAN WU¹, ELENA YAZHENSKIKH¹, KLAUS HACK², MICHAEL MÜLLER¹

¹*IEK-2, Forschungszentrum Jülich, Germany*

²*GTT Technologies, Herzogenrath, Germany*

ABSTRACT

Viscosity is a very important factor in determining the optimum operating conditions for slagging gasification, in which many processes are related to the slag viscosity, such as the particle sticking (or droplet sticking), slag flow and slag tapping that may lead to concerns about process reliability and safety. In the framework of the HotVeGas project, a new database, the so called HotVeGas oxide database, is developed for the modelling of thermochemical and thermophysical properties of ash and slag in a high-temperature gasification process. Based on the modified associate species model used in the HotVeGas Oxide database for the description of liquid phase, a novel viscosity model has already been developed for the system $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO-MgO-Na}_2\text{O-K}_2\text{O}$. The model is a structurally-based model, in which the viscosity is linked to the type and distribution of species, as well as the connectivity of species. The model parameters optimized by more than 8500 reliable experimental points give a good description of the lubricant effect as well as the charge compensation effect.

The current task is to introduce the components FeO and Fe_2O_3 to the system $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO-MgO-Na}_2\text{O-K}_2\text{O}$, to form an eight-component system. With the same principle, the viscosity is correlated to the type and distribution of species, as well as the connectivity of species. Besides the lubricant effect and amphoteric effect, another challenge for this eight-component system is to describe the redox reaction of Fe^{2+} and Fe^{3+} , in which the structural roles of Fe^{2+} and Fe^{3+} to viscosity are different. If the model is unable to describe the redox reaction, it will be only valid over a limited range of temperature and composition. However, the current model allows a good description of the redox reaction by using the Fe^{2+} based associate species as well as the Fe^{3+} based associate species, whose distribution is strongly dependent on the partial pressure of oxygen. The corresponding new model parameters are being optimized. The first calculated data are in good agreement with experimental data.

Due to the effective consideration of the internal structure of molten slags, the model is capable of predicting the viscosity over a wide range of temperature and composition by using only one set of model parameters, all of which have clear physico-chemical meaning. In addition, the current model is used to produce the three-dimensional viscosity surface, which can show a complex viscosity behaviour over more than three components. It is an application-oriented visualization of viscosity, which may be used to find optimum operating conditions for slagging gasification.